Indian J. Phys. **70B** (5), 385–390 (1996)

IJP B
— an international journal

Electron capture by protons from the outer shell of Na and K

Bablu Bhattacharjee*, Ananda Mohon Basu† and N C Deb+

*Bangabassi College School, 8/1, Santosh Mitra Square, Calcutta-700 012, West Bengal, India

†Department of Physics, Jadavpur University, Jadavpur, Calcutta-700 032, West Bengal, India

+Department of Theoretical Physics, Indian Association for the Cultivation of Science, Jadavpur, Calcutta-700 032, West Bengal, India

Received 14 May 1996, accepted 10 July 1996

Abstract : First order target continuum distorted wave approximation has been used to calculate integrated cross sections for electron capture by protons from the outer shell of Na and K. The 3*s* state of Na and 4*s* state of K are constructed by using the Roothaan-Hartree-Fock wavefunctions. The orbital energies and the effective charges of valence electrons are taken accordingly. Computed total cross sections for electron capture from these states into the 1*s* and 2*s* states of H are presented and compared with other available results.

Keywords : Charge transfer, proton impact

PACS No. : 34.70.+e

1. Introduction

There have been extensive calculation of electron capture by heavy particles from the *K*-shell of a large variety of atomic targets. Most of them involve hydrogen and helium as targets for several reasons. One important reason is that they only have *K*-shell electrons whose wave functions are known either exactly or to a good approximation. Calculations involving targets of higher nuclear charges also exist but they are mostly restricted to capture from *K*-shell. In recent years, some calculations have been reported predicting capture cross sections from *L*- and *M*-shells of a target atom. Jakubassa-Amundsen [1] reported electron capture cross sections by protons from *L*-shell of Ar. She found that the contributions from 2*s* and 2*p* initial states are larger than those from 1*s*-state and more importantly, $2p_0$ contributions are larger than those from the 2*s*-state. In a 63-state couple channel calculation, Singhal and Bransden [2] improved their earlier results [3] of capture

cross sections from 3*s*-state of Na into 1*s*, 2*s*, 2*p* states of H upto 50 keV. Throughout this energy range, they found that contributions from 2*p* captured state are consistently higher than those from 1*s* and 2*s* states and around the low energy peak, contributions from $n = 2$ levels (captured) are dominant. Very recently, Basu Chaudhury and Sural [4] employed the wave treatment of impulse approximation to calculate capture cross sections from the outer shells of alkali metals into 1*s*, 2*s* and 2*p* states of H. They reported cross sections for Na, K, Rd and Cs for the energy range 50-500 keV. At the matching energy of 50 keV, reported results of these two calculations [2,4] are quite different. The results of Singhal and Bransden [2] for all the three captured states (1*s*, 2*s* and 2*p*) are higher than those of Basu Chaudhury and Sural [4] by about a factor of 5. Another difference is that the results of Basu Chaudhury and Sural [4] decrease as the n and l values increase, whereas the results of Singhal and Bransden [2] show 2*p* cross sections are higher than those of 1*s* and 2*s* results and 2*s* contribute the least.

In the present calculation, we employ the first order target continuum distorted wave (TCDW1) approximation to calculate cross sections for electron capture by protons from the outer shell of one-valence electron target atoms in the various *s*-states of H. In section 2, we present a brief account of the TCDW1 approximation followed by results and discussions is section 3.

2. TCDW approximation

Following Crothers and Dunseath [5], the full target continuum distorted (TCDW) amplitude is given by

$$T = \left\langle \xi_f^{(-)} \middle| \left(1 + [H - E]^{\dagger} g_x^{(+)}\right) V_i \middle| \psi_i \right\rangle \tag{1}$$

$$= T^{(1)} + T^{(2)}, \tag{2}$$

where the first order term (TCDW1) is given by

$$T^{(1)} = \left\langle \xi_f^{(-)} \middle| V_i \middle| \psi_i \right\rangle \tag{3}$$

with $$\left|\xi_f^{(-)}\right\rangle = \phi_f(r_p)\, \exp(i\boldsymbol{K}_f.\boldsymbol{R}_P)\, N^*(\nu_T)\, {}_1F_1(-i\nu_T;1;-iv r_T - iv.r_T),$$

$$\left|\psi_i\right\rangle = \phi_i(r_T)\, \exp(i\boldsymbol{K}_i.\boldsymbol{R}_T),\ \nu_T = z_T/v. \tag{4}$$

ϕ_i, $\boldsymbol{K}_i$ and ϕ_f, $\boldsymbol{K}_f$ are bound states and momentum vectors in the initial and final channels.

Here we note that in the present model, the initial state is taken to be a travelling atomic orbital while the final state is represented by a TCDW function. In our calculations, we neglected the second order term $T^{(2)}$. In the full peaking approximation, $T^{(2)}$ has been shown [5] for *s*-*s* transition to be of the order of $(Z_p/v)^2$ and hence can be neglected comparing with $T^{(1)}$ which is of the order of (Z_p/v).

$T^{(1)}$ has been evaluated analytically for arbitrary initial (n, l, m) and final (n', l', m') bound states by Deb [6]. We use this analytic method to derive the transition amplitude for electron capture by protons from the $3s$ (3, 0, 0) state of Na and $4s$ (4, 0, 0) state of K into the $(n', 0, 0)$ state of H. The expression for $T^{(1)}$ is then given by

$$T^{(1)} = N(v)\, I\, \tilde{I} \tag{5}$$

with

$$I = \int d\boldsymbol{r}_T \exp(i\boldsymbol{Q}.\boldsymbol{r}_T)\, \phi_i(\boldsymbol{r}_T)\, F(i\nu_T;\, 1\,;\, iv r_T + i\boldsymbol{v}.\boldsymbol{r}_T), \tag{6}$$

$$\tilde{I} = \int d\boldsymbol{r}_P \exp(-i\tilde{\boldsymbol{Q}}.\boldsymbol{r}_P)\, \phi_f(\boldsymbol{r}_P)\, V_i(\boldsymbol{r}_P). \tag{7}$$

where $\boldsymbol{Q} = \boldsymbol{k}_i - \boldsymbol{k}_f - \boldsymbol{v}/2$, $\tilde{\boldsymbol{Q}} = \boldsymbol{k}_i - \boldsymbol{k}_f + \boldsymbol{v}/2$, $\boldsymbol{k}_i = \mu\boldsymbol{v}_i$, $\boldsymbol{k}_f = \mu\boldsymbol{v}_f$, and $\mu = M_P M_T/(M_P + M_T)$. Here $M_T(M_P)$ are the target (projectile) masses and v is the projectile velocity. Since the bound states in the final channel are hydrogenic, the evaluation of the integral $\tilde{I}$ is exactly the same as given by Deb [6] and we have

$$\tilde{I} = -4\pi(2i)^{l'} l'!\, \tilde{Q} Y_{l'm'}(\hat{\tilde{Q}}) A(n', l', \lambda_f) \sum_{k=0}^{n'-l'-1} B(n', l', k, \lambda_f) \sum_{r'=0}^{[k/2]} C(k-1, l', r') \times \frac{\lambda_f^{k-2r'}}{\left[\lambda_f^2 + \tilde{Q}^2\right]^{k+1-r'}}, \tag{8}$$

where $\lambda_f = 1/n'$ with n' is the principal quantum number of the Final Capture Channel.

We construct the initial bound states ϕ_i as the $3s$-states of Na and $4s$-states of K by using the Roothaan-Hartree-Fock atomic wave functions [7] :

$$\begin{aligned}\phi_{3s}(\mathrm{Na}) = {} & 0.03527\, \kappa_1^{(11.0123)}(r_T) + 0.00121\, \kappa_3^{(12.6601)}(r_T) \\ & - 0.01889\, \kappa_3^{(8.36156)}(r_T) - 0.06808\, \kappa_3^{(5\,73805)}(r_T) \\ & - 0.09232\, \kappa_3^{(3\,61287)}(r_T) + 0.00076\, \kappa_3^{(2\,25096)}(r_T) \\ & + 0.40764\, \kappa_3^{(1.11597)}(r_T) + 0.64467\, \kappa_3^{(0.71028)}(r_T), \end{aligned} \tag{9a}$$

$$E_i^{\mathrm{RHF}} = -0.18210, \quad Z_T^{\mathrm{eff}} = 1.810470 \tag{9b}$$

and

$$\begin{aligned}\phi_{4s}(\mathrm{K}) = {} & -0.01825\, \kappa_1^{(19\,13500)}(r_T) + 0.00031\, \kappa_1^{(31.52500)}(r_T) \\ & - 0.00899\, \kappa_2^{(16.49860)}(r_T) + 0.06350\, \kappa_2^{(7.674100)}(r_T) \\ & + 0.05015\, \kappa_3^{(6.685080)}(r_T) - 0.11346\, \kappa_3^{(4.041020)}(r_T) \\ & - 0.11474\, \kappa_3^{(2.669190)}(r_T) - 0.03065\, \kappa_4^{(2\,597940)}(r_T), \\ & + 0.05190\, \kappa_4^{(0.562030)}(r_T) + 0.33431\, \kappa_4^{(1.290170)}(r_T) \\ & + 0.70417\, \kappa_4^{(0.766410)}(r_T), \end{aligned} \tag{10a}$$

$$E^{\mathrm{RHF}} = -0.14739, \quad Z_T^{\mathrm{eff}} = 2.17175 \tag{10b}$$

with $\kappa_k^{ak} = N_k\, r_T^k \exp(-a_k r_T)\, Y_{00}(\Theta, \Phi)$

and the effective target charge for the two target atoms (Na and K) are choosen following Belkic´*et al* [8].

The integral I in eq. (6) can then be expressed as an algebriac sum of the type integrals

$$I_k = \int d\boldsymbol{r}_T \exp(i\boldsymbol{Q}.\boldsymbol{r}_T)\, r_T^{k-1} \exp(-a_k r_T)\, {}_1F_1\,(iv_{Tr};\, 1\,;ivr_T + i\boldsymbol{v}.\boldsymbol{r}_T). \quad (11)$$

Using the analytic treatment of Deb [6], the integral in eq. (11) can be evaluated to

$$I_k = \sum_{\mu=0}^{[k/2]} \frac{(-1)^\mu\, k!(k-\mu)!\alpha^{k-2\mu} 2^{k-2\mu} G^{-N}}{\mu!(k-2\mu)!}\; {}_2F_1(-N\,;\, iv_T : 1\,;\, H/G) \quad (12)$$

with $G = Q^2 + a_k^2,\ H = 2(ia_k v - \boldsymbol{Q}.\boldsymbol{v}),\ N = k - \mu + 1.$

Since the integer N is always positive, the Gauss Hypergeometric function in eq. (12) is a terminating series. The functions A, B and C in eq. (8) and other related parameters are given by

$$A(n,l,\lambda) = \left\{\frac{(2\lambda)(n-l-1)!}{2n[(n+l)!]^3}\right\}^{1/2} (2\lambda)^l,$$

$$B(n,l,k,\lambda) = \frac{(-1)^{k+2l+1}\,[(n+l)!]^2\,(2\lambda)^l}{(n-l-1)!\,(2l+1+k)!\,k!},$$

$$C(k,l,r') = \frac{(-1)^{r'}\,2^{k+l+1-2r'}\,(k+1)!\,(k+l+1-r')!}{(k+1-2r')!\,r'!}.$$

Atomic units are used throughout the calculation.

3. Results and discussion

Applying the theoretical model described in the previous section, we have calculated the total capture cross sections from $3s$ state of Na and $4s$ state of K into $1s$ and $2s$ state of atomic hydrogen. In Table 1, we present capture cross sections from $3s$ state of Na of $4s$ state of K into $1s$ state of H. We also present the corresponding results of Basu Choudhury and Sural [4]. We notice that in the lower energy region, our results are higher than those of Basu Choudhury and Sural [4] by almost a factor of two for both the targets whereas they tend to agree with each other in the high energy region. Our cross sections for capture into $2s$ state of hydrogen are presented in Table 2 together with the results of Basu Choudhury and Sural [4]. Unlike the case of capture into $1s$ state, here our results are consistently higher than those of Basu Choudhury and Sural [4] by a factor of two to four. It is interesting to note that both the impulse approximation (used by Basu Choudhury and Sural) and the present TCDW1 approximation are basically single channel distorted wave

methods. The results obtained by these two approximations tend to differ significantly. One important reason may, however, be the choice of wavefunctions used in two calculations.

Table 1. Total cross sections for ground state electron capture for p + Na($3s$) and p + K($4s$) systems in units πa_0^2. BCS represent the results of Basu Choudhury and Sural [4]. $a(-b)$ stands for $a \times 10^{-b}$.

	Na		K	
Energy (keV)	Present	BCS	Present	BCS
100	2.63 (– 3)	1.00 (– 3)	1.20 (– 3)	5.51 (– 4)
150	6.20 (– 4)	3.35 (– 4)	2.38 (– 4)	1.52 (– 4)
200	2.18 (– 4)	1.34 (– 4)	7.22 (– 5)	5.30 (– 5)
250	8.15 (– 5)		2.95 (– 5)	
300	3.65 (– 5)		1.30 (– 5)	
350	1.83 (– 5)		6.02 (– 6)	
400	1.02 (– 5)		2.73 (– 6)	
450	5.87 (– 6)		1.50 (– 6)	
500	3.74 (– 6)	3.56 (– 6)	1.01 (– 6)	9.55 (– 7)

Table 2. Same as in table 1 but for capture into 2s-state.

	Na		K	
Energy (keV)	Present	BCS	Present	BCS
100	4.98 (– 4)	8.27 (– 5)	1.99 (– 4)	4.34 (– 5)
150	1.31 (– 4)	2.41 (– 5)	5.02 (– 5)	1.06 (– 5)
200	5.04 (– 5)	1.03 (– 5)	2.16 (– 5)	3.68 (– 6)
250	2.19 (– 5)		8.22 (– 6)	
300	1.01 (– 5)		4.18 (– 6)	
350	5.21 (– 6)		2.18 (– 6)	
400	2.72 (– 6)		1.11 (– 6)	
450	1.67 (– 6)		6.33 (– 7)	
500	1.01 (– 6)	2.91 (– 7)	3.61 (– 7)	8.05 (– 8)

Basu Choudhury and Sural used the wavefunction given by Hart and Goodfriend [9] and we used the Roothan-Hartree-Fock wavefunctions. The present method can calculate cross sections for capture into an arbitrary s-state. However, we have checked that contributions from capture into 3s-state of hydrogen are at least two order of magnitude smaller than the contributions from capture into 1s-state. The present method is not sufficient to calculate contributions from capture into higher angular momentum states such as 2p-state. For this case, one need to consider the second order term (TCDW2) as well. However, with the present choice of wavefunction for the target atoms and considering the complicated

multidimensional integrals involved [5], the calculation of TCDW2 term might not be worthdoing. The results of $2p$ captured states reported by Basu Choudhury and Sural [4] also supports this claim.

4. Summary

A single channel distorted wave approximation is used to calculate the electron capture cross sections by protons from $3s$-state of Na and $4s$-state of K into $1s$ and $2s$ states of hydrogen. Roothan-Hartree-Fock wavefunctions are used for the target atoms. It is found that the cross sections obtained by our method are significantly higher than those obtained by other available methods. More accurate calculations and measurements are needed to resolve this discrepancy.

Acknowledgments

One of us (NCD) is supported by the Department of Science and Technology, Government of India, through the research grant no. SP/S2/K-01/93.

References

[1] D H Jakubassa-Amundsen *Z. Phys.* **A316** 161 (1984)

[2] R Singhal and B H Bransden *J. Phys.* **B20** 4815 (1987)

[3] R Singhal and B H Bransden *J. Phys.* **B20** L127 (1987)

[4] K Basu Choudhury and D P Sural *J. Phys.* **B25** 853 (1992)

[5] D S F Crothers and K M Dunseath *J. Phys.* **B20** 4115 (1987)

[6] N C Deb *Phys. Rev.* **A38** 1202 (1988)

[7] E Clementi and C Roetti *At. Data Nucl. Data Tables* **14** 177 (1974)

[8] Dz Belkić, R Gayet and A Salin *Phys. Rep.* **56** 279 (1979)

[9] G A Hart and P L Goodfriend *J. Chem. Phys.* **53** 448 (1970)